Temperature-driven dynamical phase transition: Spin reorientation in antiferromagnetism

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(Received 5 March 2003; revised manuscript received 16 October 2003; published 14 May 2004)

Using self-consistent quantum mean field theory, a spin reorientation transition (SRT) in antiferromagnetism (AFM) is found and the temperature-driven transition is investigated. Both the critical anisotropy and magnetization gap are quantitatively studied as a function of temperature. This SRT in AFM could be verified by x-ray magnetic linear dichroism experiments, and the existence would also support the key role of the dipolar interaction in AFM.

DOI: 10.1103/PhysRevB.69.172403 PACS number(s): 75.70.−i

Antiferromagnetism (AFM) materials in the magnetic ultrathin film subject was widely researched for the applications in exchange bias.[1,2] One of the most important findings was the antiferromagnetic domain (AFMD) observed in epitaxial thin films by the polarization-dependent x-ray magnetic linear dichroism (XMLD) spectra microscopy.[3,4] Furthermore, rather than the extrinsic origins previously argued such as defects,[5,6] the possible intrinsic mechanism of AFMD was attributed to the competition between anisotropy and dipolar interaction.[7]

In the thin ferromagnetic (FM) films, spin reorientation transition (SRT), i.e., magnetization switching from perpendicular to in-plane at a temperature below the Curie temperature (T_C), has been exhaustively studied.[8] The ferromagnetic SRT was experimentally found with dependence on both temperature and film thickness[9–11] and theoretically derived from the translational symmetry broken in the perpendicular direction of a magnetic film.[12–16] It has been established that the dipole interaction plays an important role in determining this quasi-two-dimensional (2D) magnetic phase behavior or spin reorientation transition. With the above considerations, it is naturally interesting to explore whether SRT exists in AFM.

In this paper by means of a self-consistent quantum molecular field theory, SRT in AFM is found, and the temperature-driven spin reorientation transition is investigated. Both the critical anisotropy and magnetization gap of sublattice are quantitatively studied as a function of temperature. This SRT in AFM could be verified by XMLD experiments, and the existence would support the key role of the dipolar interaction in AFM.

The model considered here is a spin-one ($S=1$) two-dimensional (2D) Heisenberg system with square lattice structure and described by the following Hamiltonian:[7]

$$H=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j+D\sum_i(\mathbf{S}_i^z)^2+U_{\mathrm{dipole}}, \tag{1}$$

$$U_{\mathrm{dipole}}=\frac{\Omega}{2}\sum_i\sum_j\left\{\frac{\mathbf{S}_i\cdot\mathbf{S}_j}{|\mathbf{l}_{ij}|^3}-3\,\frac{[\mathbf{S}_i\cdot\mathbf{l}_{ij}][\mathbf{S}_j\cdot\mathbf{l}_{ij}]}{|\mathbf{l}_{ij}|^5}\right\}, \tag{2}$$

where $D(>0)$ is the single-ion easy-plane anisotropy, U_{dipole} the dipole-dipole interaction, and $\Omega=(gu_B)^2/a^3$ (g the Lande factor, u_B the Bohr magneton, a the lattice constant) is magnetic dipolar interaction constant, $\mathbf{l}_{ij}$ is the lattice vector (in units of a) between spin $\mathbf{S}_i$ and spin $\mathbf{S}_j$. To derive the temperature-dependent magnetization, we use the quantum mean-field approach[16]

$$H=\sum_i H_i,\quad H_i=D_i(\mathbf{S}_i^z)^2+\mathbf{S}_i^zA_z+\mathbf{S}_i^xA_x, \tag{3}$$

where A_x and A_z are the mean fields defined as follows:

$$A_x=-nJM_x+\Omega M_x g_x, \tag{4}$$

$$A_z=-nJM_z+\Omega M_z g_z, \tag{5}$$

in which n is the number of nearest neighbors, M_x and M_z are the x and z components of the averaged magnetization (the y component of the averaged magnetization can be taken to be zero). It is noticed that the lattices are divided into two sublattices with average magnetization $(-1)^{lx+ly}M_x$, $(-1)^{lx+ly}M_z$ separately in the AFM system. So g_x and g_z are expressed with the following lattice sums:

$$g_x=\sum_{lx,ly}(-1)^{lx+ly}\frac{l_y^2-2l_x^2}{\{l_x^2+l_y^2\}^{5/2}}, \tag{6}$$

$$g_z=\sum_{lx,ly}(-1)^{lx+ly}\frac{l_x^2+l_y^2}{\{l_x^2+l_y^2\}^{5/2}}, \tag{7}$$

where summation of Eqs. (6) and Eq. (7) can be carried out precisely by means of the Ewald summation technique.

The effective Hamiltonian can be diagonalized exactly in the representation of S^2 and S^z eigenstates by the numerical method.[16] In the case of spin-one ($S=1$), there are three energy eigenvalues, and correspondingly three eigenvectors. Let us denote the three energy eigenvalues of H_i as ϵ_l and the corresponding three eigenvectors as $|\psi_l\rangle$, then the following self-consistent equations are obtained for the averaged magnetization M_x and M_z:

$$M_x = \overline{S_x}, \tag{8}$$

$$M_z = \overline{S_z}. \tag{9}$$

$\overline{S_x}$ and $\overline{S_z}$ are the ensemble averaged values defined as follows:

$$\overline{S_x} = \frac{\sum_l \langle \psi_l | \mathbf{S}^x | \psi_l \rangle e^{-\beta \epsilon_l}}{\sum_l e^{-\beta \epsilon_l}} \; (l=1,2,3), \tag{10}$$

$$\overline{S_z} = \frac{\sum_l \langle \psi_l | \mathbf{S}^z | \psi_l \rangle e^{-\beta \epsilon_l}}{\sum_l e^{-\beta \epsilon_l}} \; (l=1,2,3). \tag{11}$$

Generically, the self-consistent Eqs. (10) and (11) have three kinds of solutions: (i) $M_x=0$, $M_z \neq 0$, (ii) $M_x \neq 0$, $M_z=0$, and (iii) $M_x \neq 0$, $M_z \neq 0$. The truly stable magnetic configuration should be the state with the lowest free energy, which can be calculated from

$$F = -kT \; In\left[\sum_l \; \exp(-\beta \epsilon_l)\right] - \frac{1}{2}(M_x A_x + M_z A_z)$$

$$(l=1,2,3) \;\; (\text{free energy}). \tag{12}$$

Thus the temperature-dependent magnetization could be calculated from the self-consistent Eqs. (10) and (11) supplemented by the minimization condition of free-energy Eq. (12). For the zero temperature case, the self-consistent equations ($M_x = \overline{S_x}$, $M_z = \overline{S_z}$) are supplemented by the minimization of energy instead of free energy.

The magnetization relationship with anisotropy at zero temperature is as follows. At first when the anisotropy is small, due to the pure long-range dipolar interaction, spins align perpendicular to the plane: $M_x=0$; $M_z=1$. When the easy-plane anisotropy value is larger than a critical reorientation value $D^*_{\text{cri}}(0)$, the anisotropy is so strong that all the spins are in plane: $M_x=1$; $M_z=0$. In fact, this phase transition is the dynamical phase transition derived from the competition between anisotropy (D) and dipolar interaction (Ω). This transition is the first order (discontinuous) transition. This reorientation in AFM at zero temperature is due to the competition between easy-plane anisotropy and dipolar interaction.[7] The long range dipolar interactions tend to align spins along the z direction in this AFM system, while the local easy-plane anisotropy tends to drive spins in plane. So for the case of a small anisotropy, the spins are out of the plane in the z direction. And with the easy-plane anisotropy increasing, spins gradually deviate away from z direction to be in plane. Once the anisotropy reaching the critical dynamical point $D^*_{\text{cri}}(0)$, all spins are in plane to minimize the total energy.

In the following, the temperature-driven SRT of the magnetization is considered. Figure 1 shows the magnetization dependence of temperature with anisotropy below and above the critical anisotropy $D^*_{\text{cri}}(0)$. For the case of the anisotropy below $D^*_{\text{cri}}(0)$, magnetization is normal as shown in the dotted line, i.e., that M_x is always zero without in-plane component and M_z continuously decreases to zero as temperature rises. However, for the anisotropy above $D^*_{\text{cri}}(0)$ case indicated by the solid line, magnetization has an obvious feature that M_x abruptly descends to zero and M_z to nonzero correspondingly. For the system with anisotropy above $D^*_{\text{cri}}(0)$, the SRT is characterized by magnetization switching from in-plane to perpendicular direction at some temperature below the Néel point. In the mean field approximation here, the spin reorientation is the first order transition (discontinuous transition), the similar behavior of which was shown in the FM case. Although the global dipole interaction in AFM is less than the one in FM, the competitions in AFM between the vertical arrangement of pair spin induced by dipole interaction of AFM and the easy in-plane from anisotropy are expected in a similar fashion in FM. Thus SRT is not only subjected to FM, but also found in the AFM system. The physical origin of SRT in AFM is analogous to that in FM.[14]

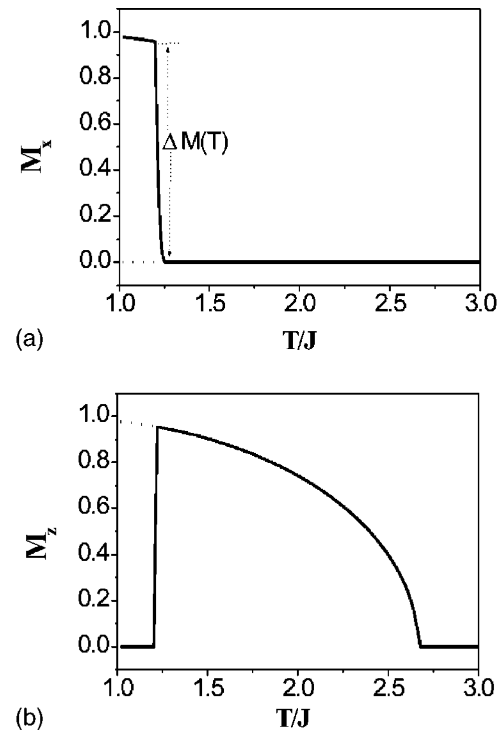

FIG. 1. (a) The magnetization M_x dependence on temperature (T). (b) The magnetization M_z dependence on temperature (T). The dotted line is for $D=0.0039$ and the solid line is for $D=0.0041$. ($J=1.000, \Omega=0.001$).

At low temperature the entropy contribution to the free energy is weak, and spins are in plane to favor the lowest energy. By contrast, as temperature increases, the entropy contribution to free energy will increase, and spins are reoriented to the perpendicular z direction to minimize the free energy. So SRT in AFM is obtained when magnetization switches from the in-plane to perpendicular direction with increasing temperature.

Figure 2 illustrates the overall magnetization of M_x vs both anisotropy and temperature. The grid line is the constant temperature (T) with variable anisotropy. At lower temperature along constant temperature line the magnetization M_x is zero for the small easy-plane anisotropy, but discontinuously

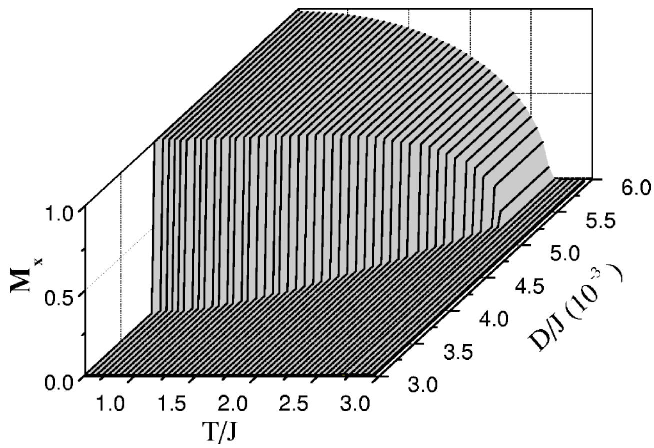

FIG. 2. The magnetization M_x vs both anisotropy (D) and temperature (T). The grid lines are the constant temperature. ($J=1.000, \Omega=0.001$).

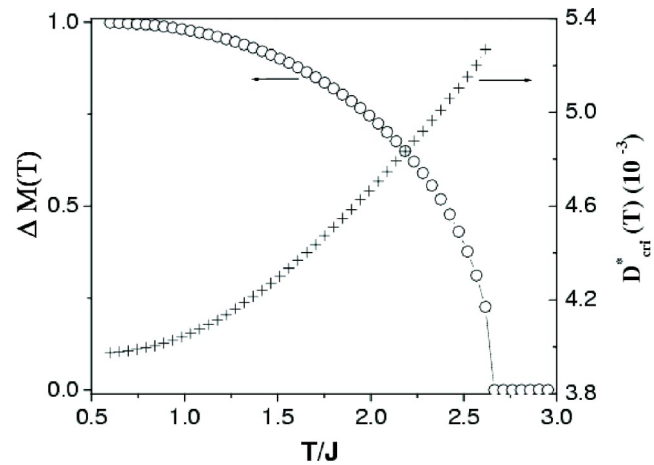

FIG. 3. Magnetization gap $\Delta M(T)$ and dynamical critical point $D^{*}_{\rm cri}(T)$ as a function of temperature. ($J=1.000, \Omega=0.001$).

jumps away from zero at the critical anisotropy $D^{*}_{\rm cri}(T)$, then remains unchanged with anisotropy above $D^{*}_{\rm cri}(T)$. The discontinuous amplitude at temperature is denoted as magnetization jump $\Delta M(T)$. The $D^{*}_{\rm cri}(T)$ increases with temperature, while $\Delta M(T)$ decreases with temperature. But the critical point will vanish at higher temperature since spins have no long range order with $M_x = M_z = 0$.

Figure 3 clearly demonstrates magnetization jump $\Delta M(T)$ and critical anisotropy $D^{*}_{\rm cri}(T)$ dependent on temperature. $\Delta M(T)$ and $D^{*}_{\rm cri}(T)$ are indicated by the circle and cross symbols, respectively. (i) At low temperature ($T<1.0$), both $\Delta M(T)(\sim 1.0)$ and $D^{*}_{\rm cri}(T)$ ($\sim 3.90\times 10^{-3}$) change smoothly. (ii) With temperature in the range (1.0, 2.6), $\Delta M(T)$ decreases rapidly from 1.0 to 0.0, and also $D^{*}_{\rm cri}(T)$ increases quickly. (iii) At high temperature the magnetization disappears, there is no phase transition anymore.

SRT in AFM system is mainly addressed based on the mean field approach model here, and several arguments are worthy to be pointed out. First, the mean-field approximation, in general, is not good for low dimensional system since the strong fluctuation specially for an system without excitation energy gap. However, the anisotropy in system induces an excitation energy gap in spin excitation spectrum, which suppresses the strong fluctuation to improve the mean-field approximation. Therefore, the picture here can keep the qualitative behavior of the SRT. Secondly, the 2D model calculated here is easily extended to the theoretical description of multilayer AFM system. And the second order SRT in AFM is possible as the case in FM if the anisotropy is different layer by layer. Third, more complex spin configurations including domain structure or vortex excitations are not considered. Also other disorders such as anisotropy fluctuations, defects or impurities in the experimental samples are omitted. To treat these subtle factors Monte Carlo calculations might be efficient. As it does not eventually violate the appearance of spin reorientation transition in the FM system where the complex spin configurations and disorder may exist, the SRT in AFM is still expected and its existence could be verified by XMLD experiments.

In summary, by self-consistent quantum mean field theory, SRT in AFM is found, and temperature-driven spin reorientation transition is investigated. Both the critical anisotropy and magnetization jump are studied as function of temperature quantitatively. This SRT in AFM could be verified by XMLD experiments, and the existence would support the key role of the dipolar interaction in AFM.

This work was supported by National Natural Science Foundation of China and 973 project (Grant No. 2002CB613504) and Shanghai Science and Technology Committee.

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